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AI Methods for Optimization Problems
• Preface •

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Preface

Zhiping Chen[1], Yu-Hong Dai[2], Tiande Guo[3] & Xinmin Yang[4]

[1]*School of Mathematics and Statistics, Xi'an Jiaotong University, Xi'an* 710049*, China;*
[2]*Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing* 100190*, China;*
[3]*School of Mathematical Sciences, University of Chinese Academy of Sciences, Beijing* 100049*, China;*
[4]*School of Mathematical Sciences, Chongqing Normal University, Chongqing* 401331*, China*

Email: zchen@mail.xjtu.edu.cn, dyh@lsec.cc.ac.cn, tdguo@ucas.ac.cn, xmyang@cqnu.edu.cn

Optimization stands as a foundational research discipline, permeating various domains such as engineering, and management, and beyond, where many problems inherently entail optimization. The development of algorithms tailored to solve optimization problems not only holds significant theoretical implications but also promises substantial practical applications.

Conventional approaches to continuous optimization predominantly rely on gradient methods, integrating analytical techniques with numerical computations to form a patterned, iterative solution framework. Combinatorial optimization, on the other hand, relies on problem-specific designs, spawning numerous research branches due to the diverse nature of problems. Challenges such as intricate design, expert knowledge dependency, and multiple constraints further complicate matters.

Conventional methods mandate the execution of an entire algorithmic pipeline for each optimization instance, thereby entailing fixed computational complexities. Once programmed, the efficiency of these algorithms, in terms of computational accuracy and complexity, remains static. Moreover, prior solving experiences offer limited transferability across instances of the same problem. However, practical scenarios often exhibit inherent similarities between problem instances or across different problems within the same domain. Traditional algorithms fail to systematically leverage these properties, let alone simultaneously address all instances of such problems.

Presently, the rapid advancement of machine learning methodologies, particularly deep learning and reinforcement learning, has catalyzed progress across various disciplines. Optimization serves as a pivotal underpinning of machine learning, with the ultimate objective often distilled into solving optimization problems—a facet of the burgeoning field of Science for AI. Conversely, AI technologies, including machine learning, have profoundly influenced scientific development, ushering in a new research paradigm—the AI for Science paradigm. Leveraging AI methods to tackle optimization problems has garnered increasing attention from scholars globally.

In 2019, the National Natural Science Foundation of China launched a significant research initiative titled "AI Methods for Optimization Problems", aimed at fostering research in this domain within China. Over the past five years, through the concerted efforts of project teams and numerous researchers, a series of noteworthy achievements have been realized. This special issue seeks to disseminate the latest research outcomes on AI methods for optimization problems, further stimulating research in this area. It spotlights exemplary research findings from the aforementioned major project groups while also welcoming submissions from other outstanding researchers. The manuscripts encompass topics ranging from AI methods for continuous optimization to multi-objective optimization, combinatorial optimization, and integer programming. Over 60 experts in AI, optimization, and related fields were invited by the guest editors to participate in the rigorous review process, with each submission undergoing scrutiny by 2–3 experts. After meticulous review spanning over a year, 11 papers were selected for inclusion in this special issue following successive stages of initial review, re-review, and final review.

Chen et al. [1] delve into L2O techniques, elucidating methods to expedite optimization algorithms, promptly estimate solutions, and even reshape the optimization problem itself, rendering it more adaptable to real-world applications. Li A Q et al. [2] propose the SimplexPseudoTree to transition the simplex method into a tree search mode while circumventing repeated basis variables. They introduce four reinforcement learning models with two actions and two rewards to tailor the Monte Carlo tree search for the simplex method, alongside establishing a new action selection criterion to refine the initial exploration's inaccurate evaluation. Li K K et al. [3] conduct further exploration to mitigate the issue of limit cycling behavior in training generative adversarial networks (GANs) through the proposed predictive centripetal acceleration algorithm (PCAA). Liu et al. [4] endeavor to sample a robust initial solution from the learned distribution to facilitate the discovery of high-quality solutions through local search. Neamatian Monemi et al. [5] tackle the intricate challenge of dock-door assignment and truck scheduling within cross-docking operations. Shi et al. [6] present a novel framework for solving various spanning tree problems by defining a Markov decision process for general combinatorial optimization problems on graphs. Wang et al. [7] propose a reinforcement learning framework to enhance cut selection in the solving process of mixed-integer linear programming (MILP). Xia et al. [8] introduce a dynamical neural network approach to address reformulated optimization problems. Yang et al. [9] introduce a gradient-based algorithm for multi-objective bi-level optimization (MOBLO), termed gMOBA, featuring fewer hyperparameters, rendering it both simple and efficient. Zeng et al. [10] propose a unified pre-training and adaptation framework for combinatorial optimization problems on graphs, leveraging the maximum satisfiability (Max-SAT) problem. Zhang et al. [11] propose a generalized framework for learning the components of AOS for one of the primary streams of EAs, namely, differential evolution.

This special issue primarily targets researchers in optimization, machine learning, AI, data mining, and related disciplines, showcasing the latest research advancements by Chinese scholars in the realm of "AI for optimization". We extend our heartfelt gratitude to the editorial board of *SCIENCE CHINA Mathematics* for their guidance and assistance throughout the publication of this special issue. Special acknowledgment is due to all the editors in the editorial office for their tireless efforts—from conceptualization to solicitation, expert invitation, review summarization, revision, finalization, and publication of the papers. We are also grateful for the diligent and meticulous review work conducted by our esteemed reviewers. Furthermore, we express our sincere appreciation to the authors who have contributed actively to this special issue, placing their trust in *SCIENCE CHINA Mathematics*. Lastly, we extend our gratitude to the readers of this special issue, hoping it will contribute to the advancement of research in this pertinent field.

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